3-Propylglutaric acid

Other names: «beta»-n-Propylglutaric acid
3-n-Propylglutaric acid
Pentanedioic acid, 3-propyl-
Inchi: InChI=1S/C8H14O4/c1-2-3-6(4-7(9)10)5-8(11)12/h6H,2-5H2,1H3,(H,9,10)(H,11,12)
InchiKey: YHJZYPZZBZPIPX-UHFFFAOYSA-N
Formula: C8H14O4
SMILES: CCCC(CC(=O)O)CC(=O)O
Mol. weight [g/mol]: 174.19
CAS: 4165-98-4

Physical Properties

Property code	Value	Unit	Source
gf	-517.44	kJ/mol	Joback Method
hf	-743.35	kJ/mol	Joback Method
hfus	24.33	kJ/mol	Joback Method
hvap	79.86	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	1.352		Crippen Method
mcvol	138.460	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
tb	674.10	K	Joback Method
tc	849.38	K	Joback Method
tf	386.42	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.20	J/mol×K	674.10	Joback Method
cpg	381.95	J/mol×K	703.31	Joback Method
cpg	390.25	J/mol×K	732.53	Joback Method
cpg	398.13	J/mol×K	761.74	Joback Method
cpg	405.59	J/mol×K	790.95	Joback Method
cpg	412.65	J/mol×K	820.16	Joback Method

cpg	419.32	J/mol×K	849.38	Joback Method
dvisc	0.0057482	Pa×s	386.42	Joback Method
dvisc	0.0013650	Pa×s	434.37	Joback Method
dvisc	0.0004314	Pa×s	482.31	Joback Method
dvisc	0.0001679	Pa×s	530.26	Joback Method
dvisc	0.0000764	Pa×s	578.21	Joback Method
dvisc	0.0000392	Pa×s	626.15	Joback Method
dvisc	0.0000222	Pa×s	674.10	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4165984&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume